

## The effect of functionalizing graphene nanosheets on adsorption of Hydroxynaphtol Blue dye, A molecular dynamics simulation

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One of the most effective methods for removing many pollutants from aqueous solutions is adsorption. Removal of particles based on adsorption is accomplished by connecting dissolved pollutants in a stream towards a solid surface. In this process, choosing an adsorbent with high selectivity over the desired pollutant is very important [1]. Occasional levels of adsorption can be increased by using auxiliary groups; in other words, the adsorbent can be modified. Today, graphene nanosheets are one of the most widely used adsorbents in the field of adsorption that can also be improved with auxiliary groups [2]. In the present study, the process of adsorption of hydroxynaphtol blue (as a dye that is a water pollutant) on pure and oxidized graphene nanosurfaces is simulated at 298 K with DL\_POLY\_2.17 simulation package. Analyzing the radial distribution function (RDF) between the dye center of mass (COM) and the graphene nanosheets demonstrates the effect of surface modification on the adsorption. As seen in Figure 1, oxidation of graphene nano surface with the combination of hydroxy and epoxy groups enhances the adsorption of the desired dye on the surface and rises the efficiency of the adsorption process. Here, hydrogen atoms of hydroxy group possess the best contribution on adsorption process.

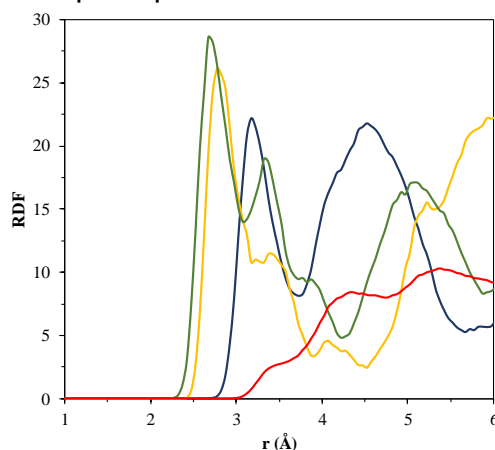


Fig. 1 RDF of dye COM and surface atoms. Green, hydrogen atom of hydroxy group; yellow, oxygen of epoxy group; blue, oxygen of hydroxy group; and red, carbon atoms of graphene nanosheet.

### References

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- [2] A. Elsagh, O. Moradi, A. Fakhri, F. Najafi, R. Alizadeh, V. Haddadi, Arabian Journal of Chemistry, **2017**, 10, S2862.